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NMR self-diffusion study of a phosphonium bis(mandelato)borate ionic liquid

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Abstract

Newly synthesised halogen-free boron based ionic liquids (hf-BILs) composed of chelated orthoborate anions and phosphonium cations have hydrolytic stability, low melting point and outstanding wear and friction reducing properties. We report here the peculiarities of self-diffusion in one representative from this class, trihexyltetradecylphosphonium bis(mandelato)borate, [P6,6,6,14][BMB], in the temperature range of its practical interest, 20-100 °C. NMR techniques demonstrated complicated diffusional behaviour-the ionic liquid can exist in one or two liquid "phases". In the low-temperature range (20-50 °C), two phases coexist where the cations, [P6,6,6,14], are contained mainly in the phase with slower diffusion coefficients while the anions, [BMB], are in the phase with faster diffusion coefficients. Cations have lower diffusion coefficients with a factor of 20 as compared with the anions, an effect which is caused by aggregation of cations into domains due to so-called "hydrophobic interaction" of their hydrocarbon chains. As the temperature rises above 60 °C, the two phases merge into one where both ions have equal diffusion coefficients. This is caused by thermal motion making the cation domains smaller in size and more easily interacting with anions. As a result, anions and cations diffuse in this high-temperature range as a pair. © 2013 the Owner Societies.

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